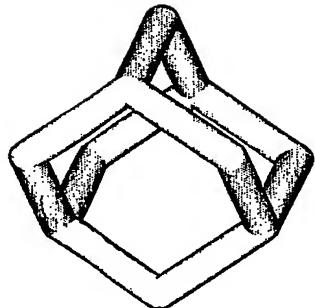
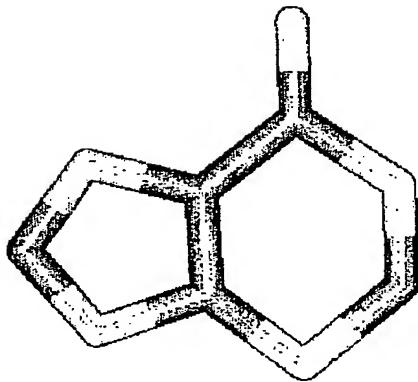


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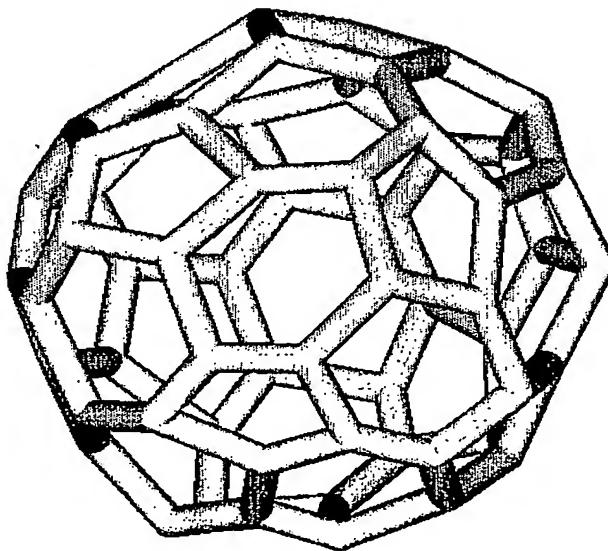
adamantane (RMSD = 0.04Å)



adenine (RMSD = 0.12Å)

FIG. 1A

FIG. 1B



fullerene (RMSD = 0.24Å)

FIG. 1C

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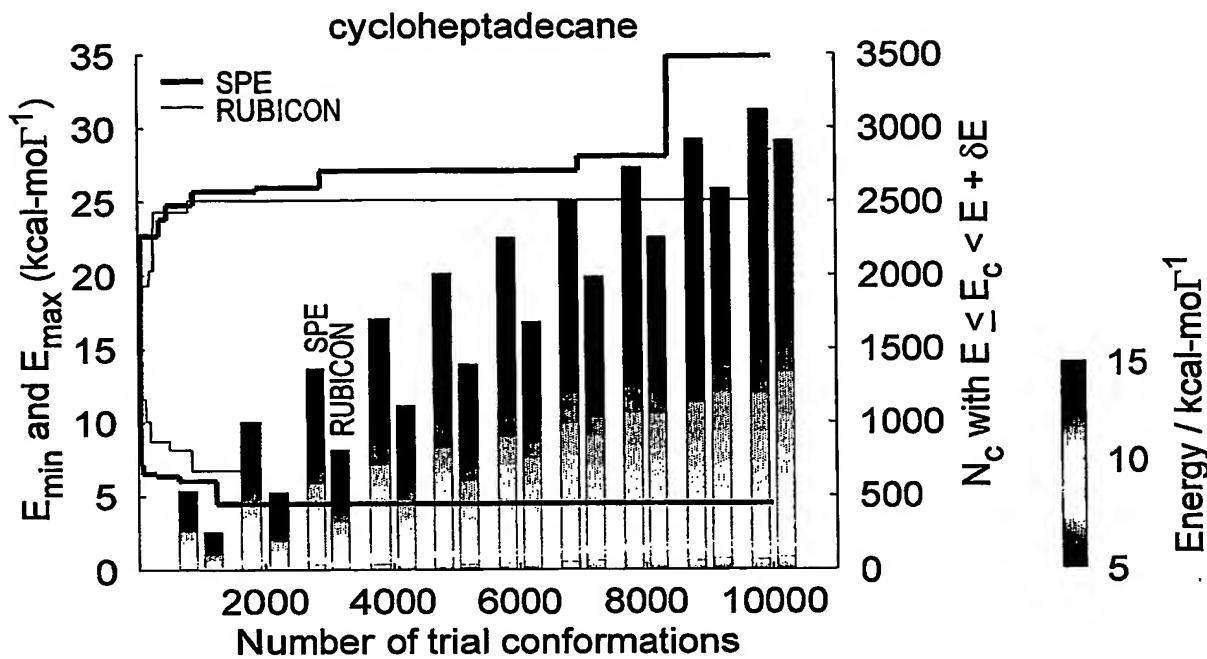


FIG.2A

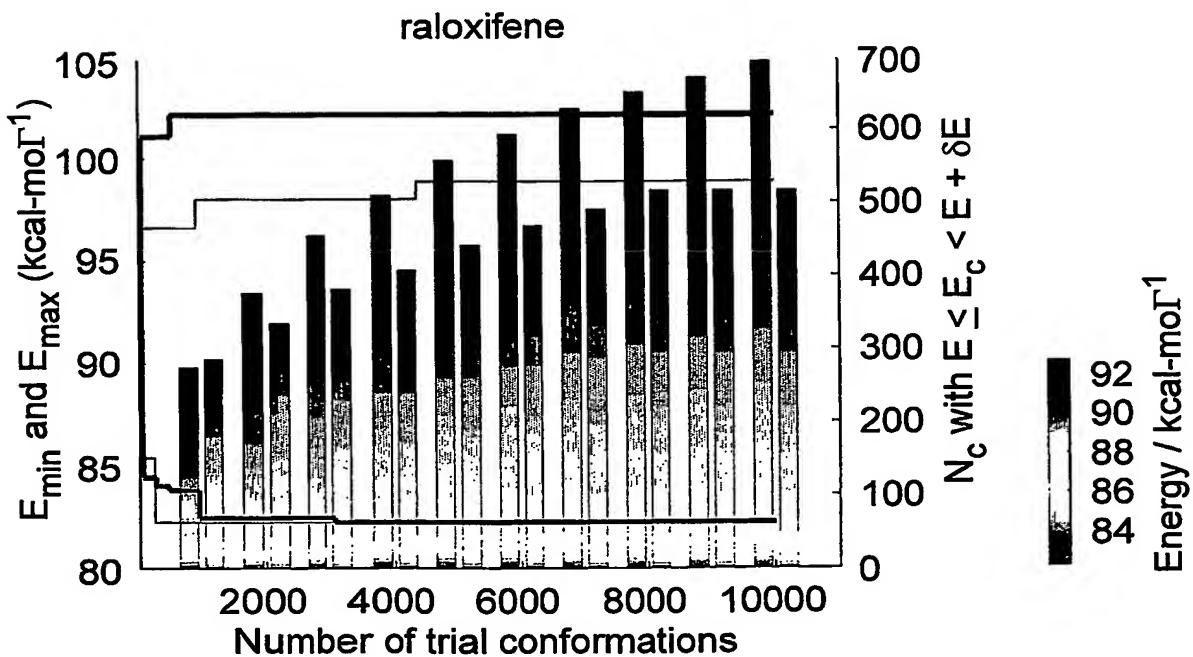


FIG.2B

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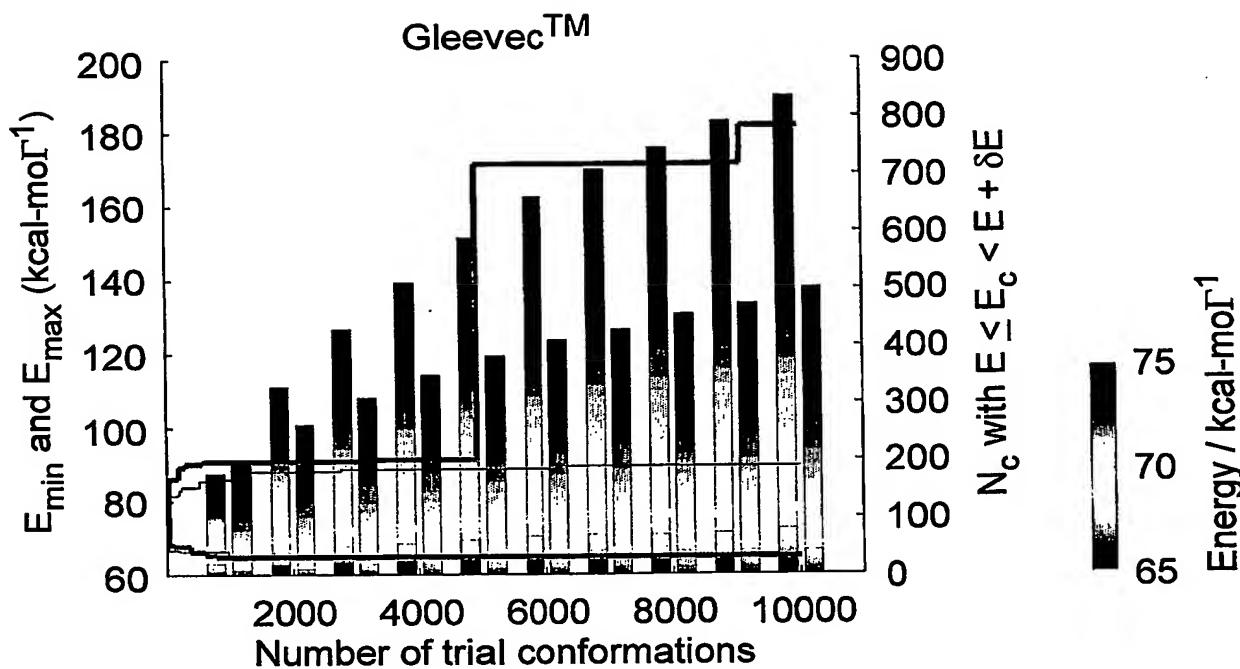


FIG. 2C

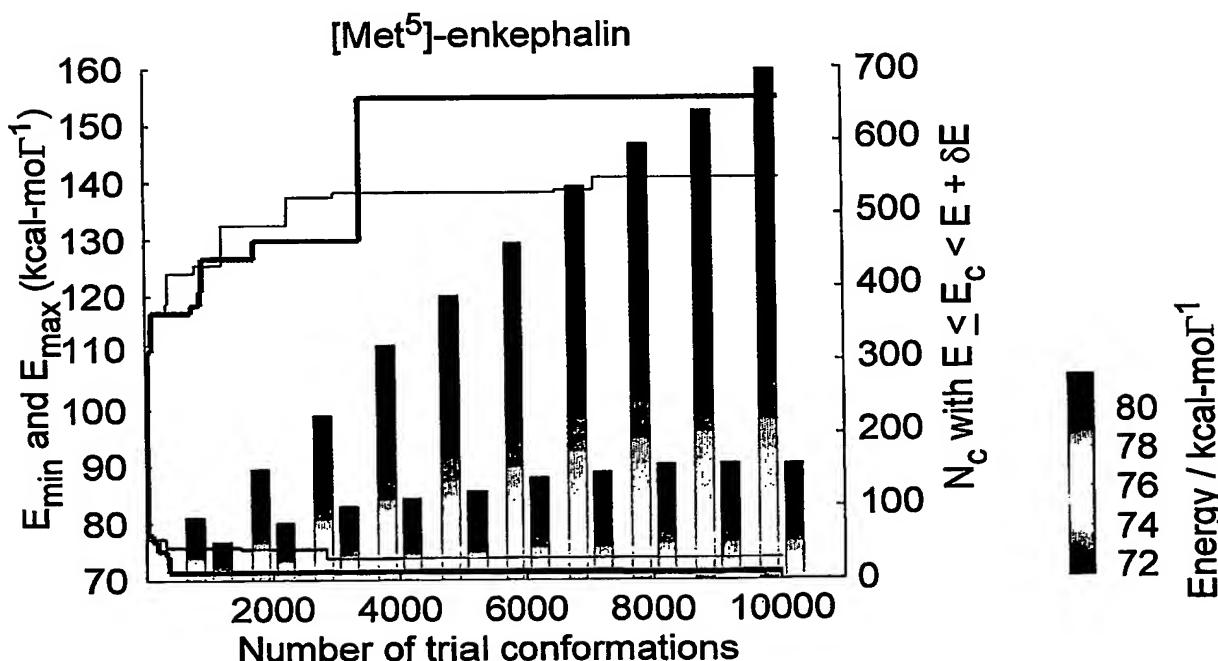


FIG. 2D

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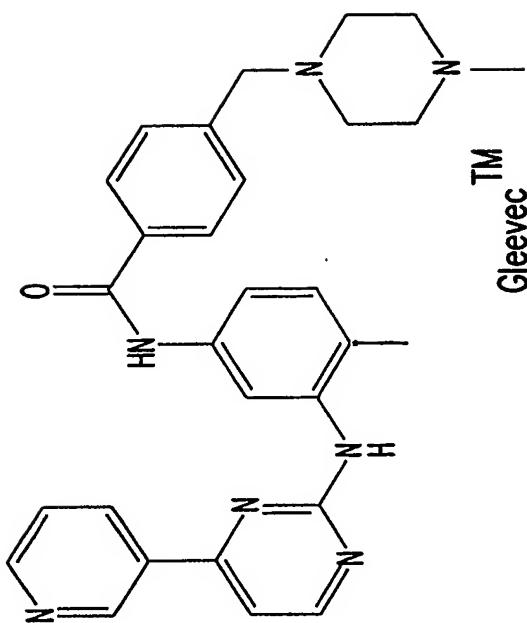


FIG. 3B

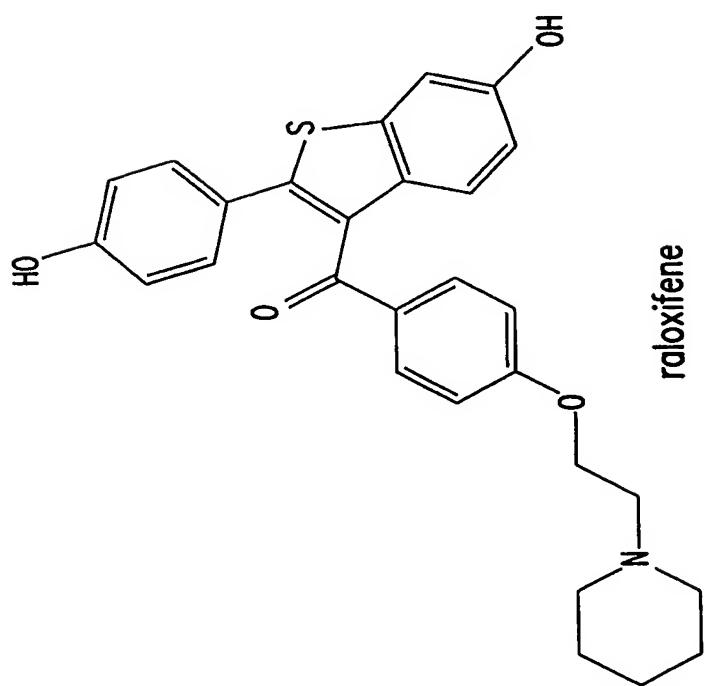
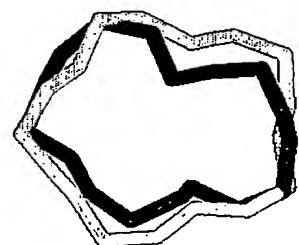


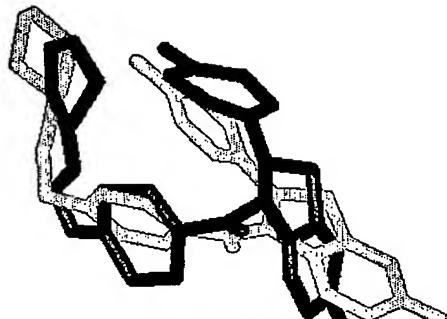
FIG. 3A

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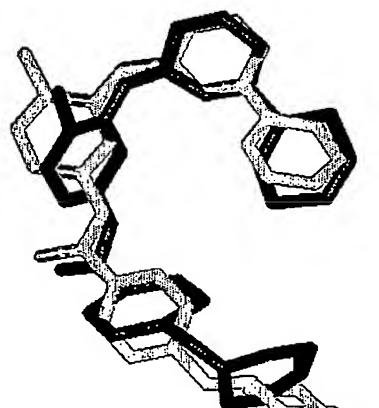
cycloheptadecane  
(RMSD=0.90Å)

FIG.3C



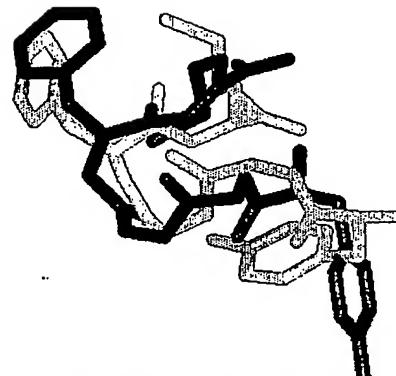
raloxifene  
(RMSD=1.51Å)

FIG.3D



Gleevec™  
(RMSD=1.69Å)

FIG.3E



[Met⁵]-enkephalin  
(RMSD=2.43Å)

FIG.3F

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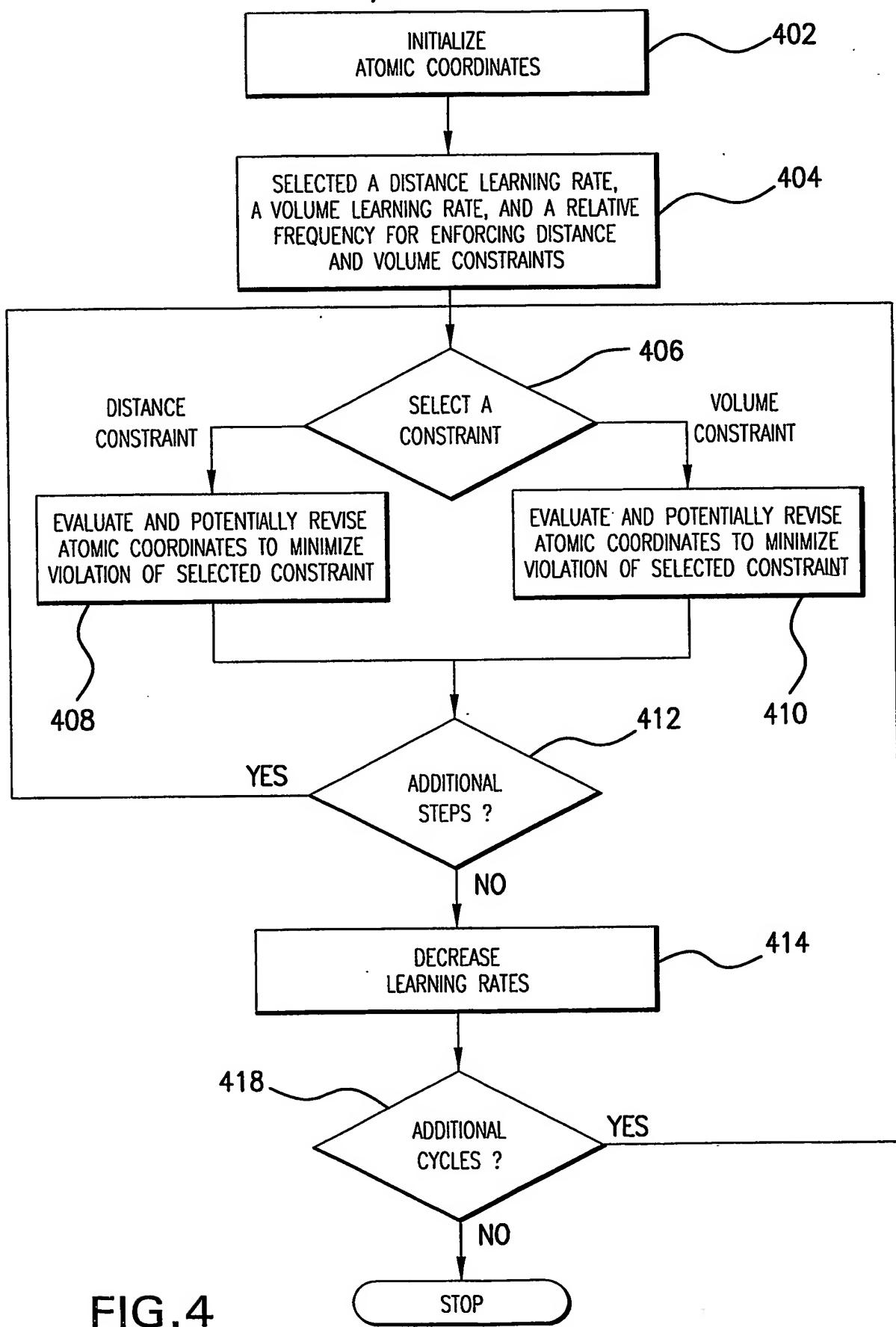


FIG.4

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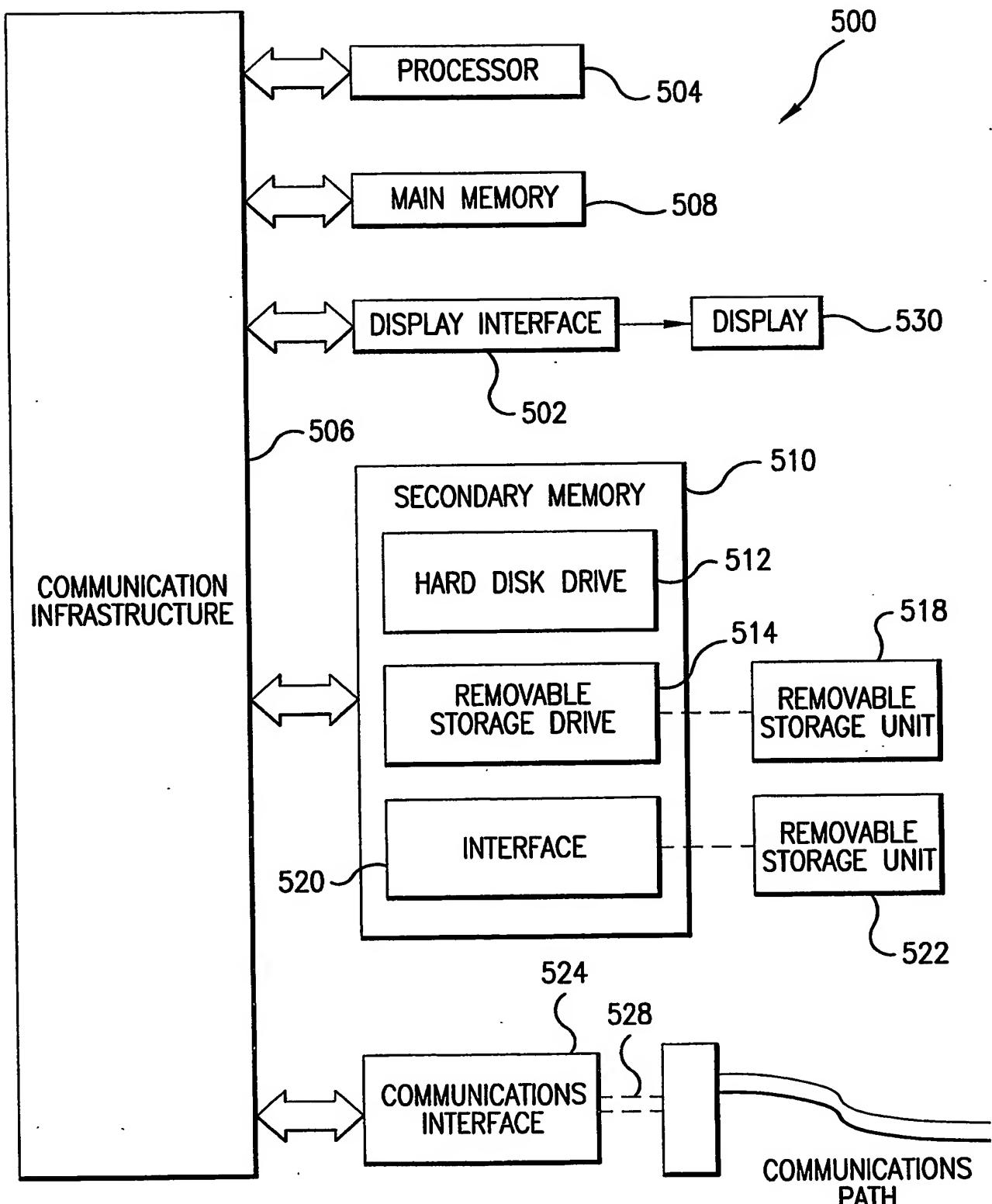


FIG. 5

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MOLECULE	$t_{\text{SPE}}$ (sec)	$t_{\text{RUBICON}}$ (sec)	$n_d^{\text{SPE}}$	$n_d^{\text{RUBICON}}$	$\dot{E}_{\text{min}}^{\text{SPE}}$ ( $\text{kcal} \cdot \text{mol}^{-1}$ )	$\dot{E}_{\text{min}}^{\text{RUBICON}}$ ( $\text{kcal} \cdot \text{mol}^{-1}$ )
cycloheptadecane	0.049	0.615	5908	4453	4.5105	4.5105
raloxifene	0.242	1.215	1915	689	82.2486	82.2486
Gleevec <sup>TM</sup>	0.261	1.677	3482	1228	64.8114	64.8482
[Met <sup>5</sup> ]-enkephalin	0.306	1.819	9995	8019	71.3763	73.8235

TABLE 1

FIG. 6